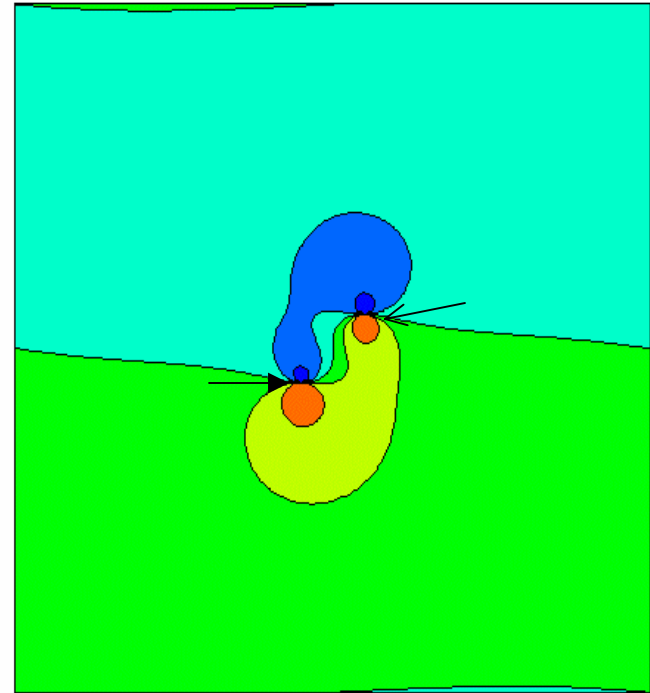


# Defect Interaction in Solids: Impact on Microstructure and Materials Properties

J. M. Rickman, Lehigh University, DMR-9975384

The presence and motion of dislocations in metals are known to affect many of their mechanical properties, including plastic response. Thus, interactions with objects that can hinder the motion of these line defects play a key role in determining how metals will deform. With this in mind, computational materials scientists have sought to understand better the mechanisms associated with dislocation pinning, especially as a result of interaction with atoms in solid solution.

The complex interplay among mobile point and line defects can perhaps best be illustrated via dynamical simulations where dislocation motion is driven, in part, by an external stress. In some regimes, solute clouds moving with dislocations form composite objects, as illustrated here. These dislocations periodically escape from the clouds and are recaptured, leading to a dynamic pinning phenomenon.



Calculated isoconcentrates for solute about two, interacting edge dislocations. In some regimes one can view these objects as composite “quasiparticles”. (The locations of the dislocations are indicated by arrows.)

Y. Wang *et al.*, Acta Mater. **48**, 2163 (2000).

J. M. Rickman *et al.*, Acta Mater. **51**, 1199 (2003)

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## Broader Impacts:

**Education** - The education of graduate students and the enhancement of the undergraduate and graduate curricula are two principal aims of this program. At present, two Ph.D. students, Cory Lowe (Physics) and Thirumalesh Bannuru (Materials Science) are working on projects involving dislocation dynamics.

We have also developed an undergraduate computational methods course for materials science majors. This program has led to various instructional materials for that course.

## Synergistic Activities:

- Co-edited (with R. LeSar) special volume of Annual Reviews of Materials Research focusing on computational materials science.
- Organized focused symposia for Spring TMS and MRS meetings.
- Service on Computer Simulation Committee of TMS (Vice-President).
- Development of a Web-based, graduate-level course on the subject of crystalline defects.